

Toward Understanding Alloying Element Vaporization during Laser Beam Welding of Stainless Steel

A comprehensive model is proposed to predict vaporization rates during welding. Predictions are compared with experimental data

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ABSTRACT. During laser beam welding of many important engineering alloys, appreciable changes in the composition and properties of the weld metal can occur due to pronounced vaporization of alloying elements from the weld pool. Currently there is no comprehensive theoretical model to predict, from fundamental principles, laser-induced metal vaporization rates and the resulting weld pool composition changes.

The velocity distribution functions of the gas molecules at various locations above the weld pool surface and the heat transfer and fluid flow phenomena in the pool have been coupled to model the rates of the vaporization of various alloying elements during laser beam welding of stainless steels. The procedure allows for computation of both the evaporation and condensation fluxes based on the equations of conservation of mass, momentum and energy applied to the vapor and the liquid phases. Computed values of the rates of vaporization of various alloying elements and the vapor composition were found to be in good agreement with the corresponding ex-

perimental values. Synthesis of the principles of gas dynamics and weld pool transport phenomena can serve as a basis for the calculation of alloying element vaporization rates during laser beam welding of alloys.

Introduction

The use of a high power density laser beam for welding leads to weld pool temperatures that are often higher than those encountered in most other welding processes. Even at modest power

densities, laser beam welding of many important engineering alloys results in significant changes in composition and properties of the weld metal (Refs. 1-4). Because of its importance, vaporization of alloying elements during welding has been investigated both experimentally and theoretically. Apart from the examination of the weld metal composition and structure to evaluate the direct effects of vaporization, much of the previous experimental work was based on in-situ monitoring of the alloying element vaporization by emission spectroscopy (Refs. 5-7). It was found that during welding of stainless steels, the dominant species in the vapor phase were iron, manganese, nickel and chromium. Eagar and Block-Bolton (Ref. 8) used calculations based on the Langmuir equation to demonstrate that iron and manganese were the most prominent vapor species in the welding environment. Although the rates calculated by the Langmuir equation have been used for the determination of the relative vaporization rates of various alloying elements, the calculated vaporization rates are generally significantly higher than the corresponding experimentally determined values at one atmosphere pressure. Even at pressures as low as 200 micrometers of Hg, the vaporization rates of pure

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shown that vaporization can significantly influence the temperature field on the pool surface. The local heat flux from the pool surface, J_h , in $J/m^2\text{-s}$ is given by

$$J_h = h\{T_l - T_g\} + \sum_{i=1}^n J_i \Delta H_i \quad (1)$$

where T_l is the local weld pool surface temperature, T_g is the ambient temperature, J_i is the vaporization flux in $kg/m^2\text{-s}$ of an element i , ΔH_i is the enthalpy of vaporization of the element i in J/kg , n is the number of alloying elements and h is the heat transfer coefficient in $J/m^2\text{-s-K}$. The heat transfer coefficient for a gas jet impinging on a surface was derived from the graphical results of Schlunder and Gnielinski (Ref. 19) and is given by the following relation:

$$h = \frac{2Pr^{0.42} Re^{0.5} k}{d} \left(1 + \frac{Re^{0.55}}{200}\right)^{0.5} \left[0.483 - 0.108 \frac{r}{d} + 7.71 \times 10^{-3} \left\{\frac{r}{d}\right\}^2\right] \quad (2)$$

where d is the diameter of the nozzle in meters, r is the radial distance on the pool surface in meters, k is the thermal conductivity of shielding gas in $J/m\text{-s-K}$ at temperature T_{av} , which is the arithmetic average of T_l and T_g , Re is the Reynolds number at the nozzle exit and Pr is the Prandtl number.

Vaporization Due to Pressure Gradient

In laser processing of the metals and alloys, the temperatures reached on the surface can be very high and often exceed the boiling point (Refs. 20, 21). For example, von Allmen (Ref. 22) determined molten pool temperatures in excess of boiling point for laser treatment of copper. Batanov, *et al.* (Ref. 23), indicated that temperatures on the surface of the laser irradiated material can be higher than the normal boiling point of the material. Paul and DebRoy (Ref. 16) and Zacharia, *et al.* (Ref. 24), have reported temperatures close to the boiling point for laser beam welding. Khan and DebRoy (Ref. 2) measured the liquid pool surface temperatures close to the boiling point from the ratio of the rates of vaporization of alloying elements. Chan and Majumdar (Ref. 12) have also reported temperatures greater than boiling point for the laser irradiation of aluminum, titanium and a superalloy. Theoretical calculations of the vaporization rates by Knight (Ref. 11) and Anisimov (Ref. 10) are based on the premise that the liquid pool surface temperatures are higher than the boiling point.

At temperatures higher than the boiling point, the pressures in the vicinity of the pool are greater than the ambient

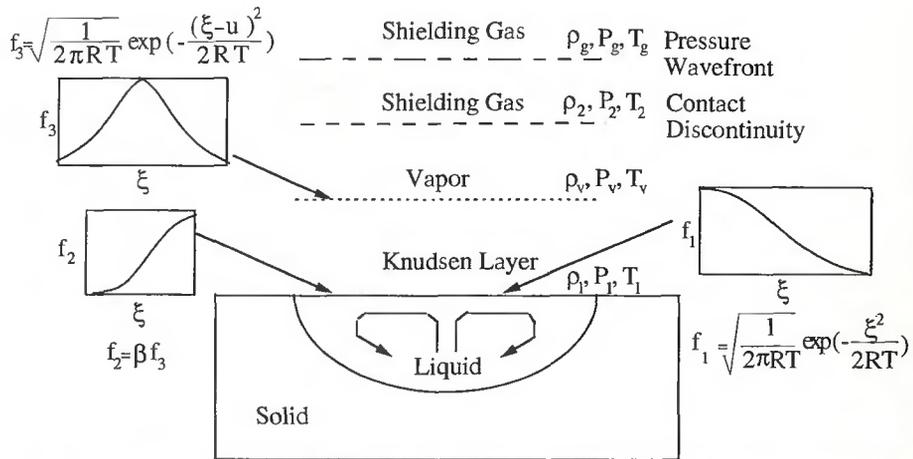


Fig. 2 — A schematic diagram of the velocity distribution junctions in the Knudsen layer and in adjacent regions.

pressure and the excess pressure provides a driving force for the vapor to move away from the surface. The velocity distribution functions of the vapor molecules escaping from the weld pool surface at various locations are shown schematically in Fig. 2. Near the weld pool surface, the molecules cannot travel in the negative direction, and as a consequence, the distribution function is half-Maxwellian. Close to the weld pool surface there exists a space of several mean free paths length, known as the Knudsen layer (Ref. 10), at the outer edge of which the velocity distribution reaches the equilibrium distribution. Here, the vapor molecules can have all possible velocities from $-\infty$ to $+\infty$, at least in principle, as observed in Fig. 2. A portion of the vaporized material condenses on the liquid surface.

The temperature T_v , density ρ_v , pressure P_v and the mean velocity of the vapor, u , at the edge of the Knudsen layer can be related to temperature, T_l , pressure, P_l , and the density, ρ_l , of the vapor at the liquid surface by treating the Knudsen layer as a gas-dynamic discontinuity. Anisimov (Ref. 10) and Knight (Ref. 11) derived expressions for the changes in the vapor density, temperature, velocity and the extent of condensation by using the velocity distribution functions presented in Fig. 2 and solving the equations of conservation of mass, momentum and translational kinetic energy across the Knudsen layer. Since the details of the procedure are available in their papers, only a summary of the results, commonly referred to as the jump conditions, are presented in Equations 3 to 5.

$$\frac{T_v}{T_l} = \left(\sqrt{1 + \pi \left(\frac{\gamma_v - 1}{\gamma_v + 1} \frac{m}{2} \right)^2} - \sqrt{\pi} \frac{\gamma_v - 1}{\gamma_v + 1} \frac{m}{2} \right)^2 \quad (3)$$

where $m = u/\sqrt{2 R_v T_v}$, $R_v = R/M_v$, R is the gas constant in $J/mole\text{-K}$, γ_v is the ratio of specific heats of the vapor, which is treated as a monoatomic gas, and M_v is the average molecular weight of the vapor in $kg/kg\text{-mole}$

$$\frac{\rho_v}{\rho_l} = \frac{T_l}{T_v} \left(\left(m^2 + \frac{1}{2} \right) e^{m^2} \operatorname{erfc}(m) - \frac{m}{\sqrt{\pi}} \right) + \frac{1}{2} \frac{T_l}{T_v} \left(1 - \sqrt{\pi} m e^{m^2} \operatorname{erfc}(m) \right) \quad (4)$$

where erfc is the complimentary error function.

The condensation factor, β , is given by

$$\beta = \left(2m^2 + 1 \right) - m \sqrt{\pi} \frac{T_l}{T_v} e^{m^2} \frac{\rho_l}{\rho_v} \sqrt{\frac{T_l}{T_v}} \quad (5)$$

The density, ρ_l , can be computed from P_l and T_l , assuming that the vapor behaves like an ideal gas. The equilibrium vapor pressure, P_l , at the pool surface is obtained from the equilibrium vapor pressure-temperature relationships of the various alloying elements.

$$\frac{P_l}{P_g} = \sum_{i=1}^n a_i \frac{P_i^s}{P_g} \quad (6)$$

where P_g is the ambient pressure, a_i is the activity of the alloying element i and P_i^s is the equilibrium vapor pressure of the pure element i at T_l and n is the number of alloying elements. Since the temperatures at the weld pool surface are very high, the activities were taken to be equal to the corresponding mole fractions. The average molecular weight of the vapor, M_v , in the Knudsen layer is given by:

$$M_v = \sum_{i=1}^n M_i \frac{a_i P_i^s}{P_l} \quad (7)$$

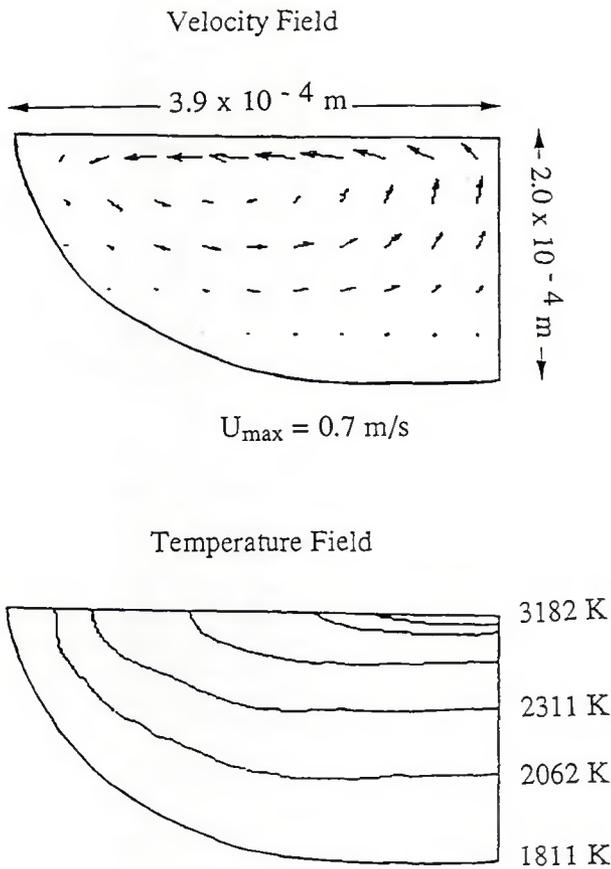


Fig. 3 — Velocity and temperature fields for a laser power of 560 W and helium gas flow rate of 6 L/min.

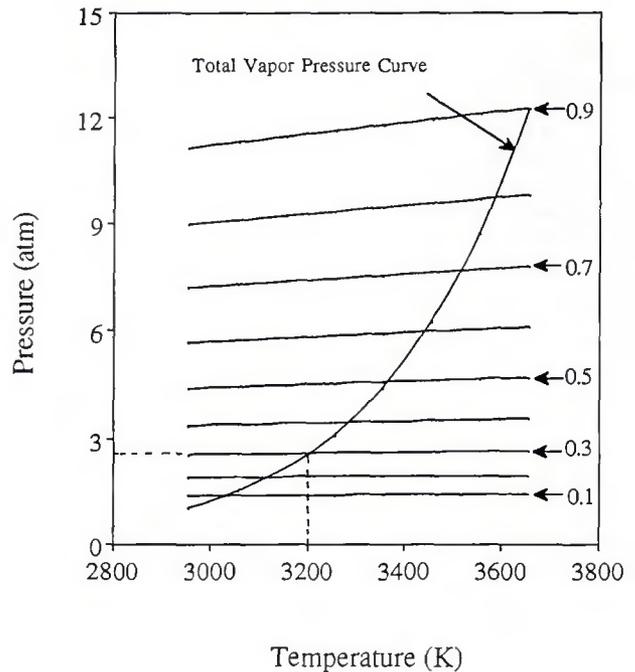


Fig. 4 — Flow state diagram for AISI 202 stainless steel in helium atmosphere. The Mach number for various lines is indicated in the figure.

where M_i is the molecular weight of species i , a_i is the activity i in the liquid metal, and P_i° is the equilibrium vapor pressure of the pure element i at T_1 . Since there are four unknowns in Equations 3 to 5, viz. T_v , p_v , β and m , it is necessary to have an additional equation to have unique values of these variables. The necessary equation is obtained by relating the pressure at the edge of the Knudsen layer to the ambient conditions. Across the Knudsen layer the vapor wavefront moves into the shielding gas, as shown in Fig. 2. The moving interface between the vapor and the shielding gas is a contact discontinuity. Across this discontinuity, the pressures are the same, i.e., $P_2 = P_v$. The pressure rise at the liquid-vapor interface propagates as a pressure wave as shown in Fig. 2. The wavefront may be treated as a pressure discontinuity, and the pressure change across the wavefront may be obtained by applying the Rankine-Hugoniot relation (Ref. 25).

$$\frac{P_2}{P_1} = \frac{P_v}{P_1} = 1 + \gamma_g M \Gamma \left(\frac{\gamma_g + 1}{4} M \Gamma + \sqrt{1 + \left(\frac{\gamma_g + 1}{4} M \Gamma \right)^2} \right) \quad (8)$$

where P_1 and P_2 are the pressures in front of and behind the wavefront, respectively. γ_g is the ratio of specific heats for shielding gas and $\Gamma = \sqrt{\gamma_v R_v T_v} / \sqrt{\gamma_g R_g T_g}$. The Mach number, M , is related to m according to the equation

$$m = M \sqrt{\frac{\gamma_g}{2}} \quad (9)$$

In Equation 8, P_1/P_g can be computed from Equation 6 for a given local surface temperature and, since $P_2 = P_v$, for an ideal gas, P_2/P_1 can be expressed as a function of m with the help of Equations 3 and 4. Thus, Equation 8 is effectively reduced to a nonlinear equation in m and can be solved iteratively or graphically to obtain m and the Mach number for a given local weld pool surface temperature. The values of T_v , p_v and β , corresponding to a local temperature T_1 can be determined from Equations 3 to 5 by using the computed value of m . The Mach number and the density ρ_v can then be used to calculate the vaporization flux, J_p , in $\text{kg/m}^2\text{-s}$, due to pressure gradient at the pool surface corresponding to a local surface temperature T_1 .

$$J_p = \rho_v M S \quad (10)$$

where S is the speed of sound in vapor at temperature T_v . Since the rate of vaporization of an alloying element will be proportional to its partial pressure over the pool, its flux, $J_{p,i}$ is given by

$$J_{p,i} = a_i \frac{P_i^\circ}{P_1} \frac{M_i}{M_v} J_p \quad (11)$$

Vaporization Due to Concentration Gradient

At the pool surface, the concentrations of the alloying elements in the vapor is considerably higher than their respective concentrations in the bulk shielding gas. The vaporization flux of an element i due to concentration gradient, $J_{c,i}$ in $\text{kg/m}^2\text{-s}$, is then defined as

$$J_{c,i} = K_{g,i} M_i \frac{a_i P_i^\circ}{RT_1} \quad (12)$$

where P_i° is equilibrium vapor-pressure of the element i over pure liquid i in atmosphere, M_i is the molecular weight of the element i in kg/kg-mole , R is the gas constant in $\text{m}^3 \text{atm/kg-mole K}$ and $K_{g,i}$ is the mass transfer coefficient of the element i in m/s . The mass transfer coefficient was derived from the graphical

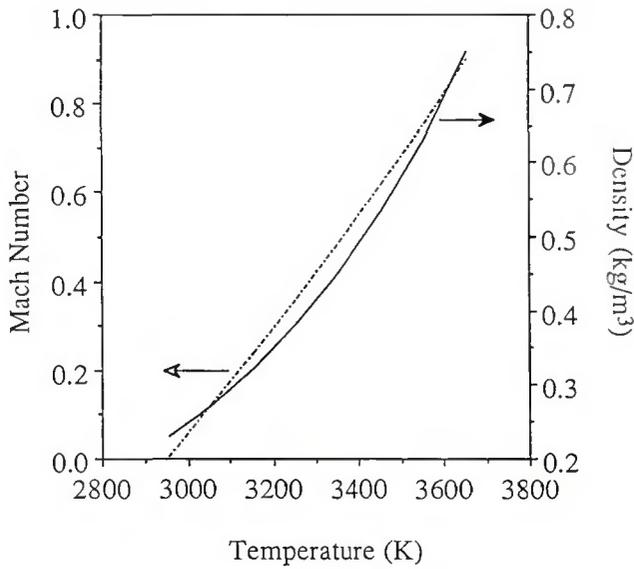


Fig. 5 — Mach number and density for AISI 202 stainless steel for various temperatures at the edge of Knudsen layer in helium atmosphere.

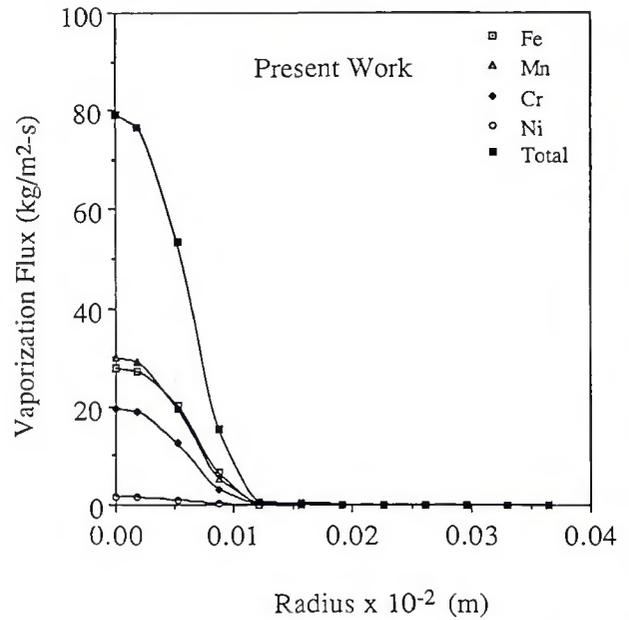


Fig. 6 — Vaporization flux for various alloying elements, and the total flux from the model presented in this paper.

results of Schlunder and Gnielinski (Ref. 19) and is given by

$$K_{r,i} = \frac{2Sc^{0.42} Re^{0.5} D \left(1 + \frac{Re^{0.55}}{200}\right)^{0.5}}{d} \left[0.483 - 0.108 \frac{r}{d} + 7.71 \times 10^{-3} \left\{\frac{r}{d}\right\}^2\right] \quad (13)$$

where d is the diameter of the nozzle in meters, r is the radial distance on the pool surface in meters, D is the diffusivity of the element in shielding gas in m^2/s at temperature T_{av} , Re is the Reynolds number at the nozzle exit and Sc is the

Schmidt number of the element at average temperature T_{av} . The total vaporization flux, J_i , for an element i is then given by

$$J_i = J_{p,i} + J_{c,i} \quad (14)$$

Results and Discussion

Velocity and Temperature Fields

When the laser beam strikes the surface of the samples, melting occurs al-

most instantaneously. For a high power density laser beam, the time required to reach steady state is very small. Zacharia, *et al.* (Ref. 24), noted that in laser beam welding quasi-steady state is achieved very quickly. Mehrabian, *et al.* (Ref. 26), showed that the time required to reach the maximum melt depth in iron for a laser power of $2 \times 10^5 W/cm^2$ is of the order of 1 ms. Thus, for almost the entire duration of a large laser pulse of several milliseconds span, the molten pool remains in a steady state. The

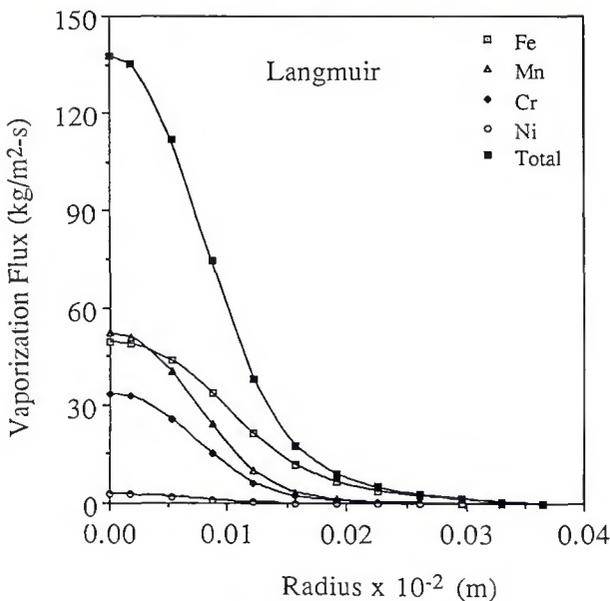


Fig. 7 — Vaporization flux for various alloying elements and the total flux computed using Langmuir equation.

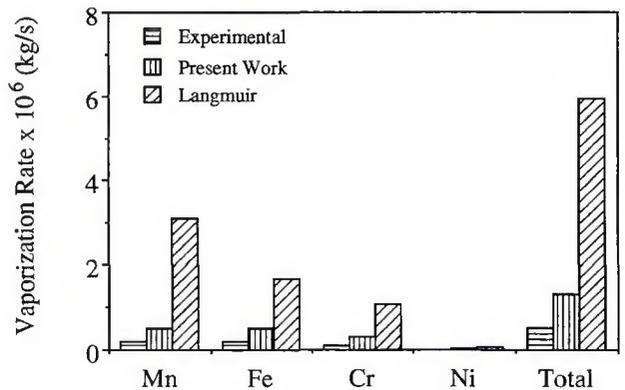


Fig. 8 — Comparison of the experimental vaporization rates with the rates calculated from the Langmuir equation and from the model presented in this paper.

Table 1— Data Used for Calculations in the Welding of AISI 202 Stainless Steel

Property/Parameter	Value
Density (kg/m ³)	7200.0
Melting point (K)	1811.0
Laser power (W)	560.0
Radius of the beam (m)	2.0×10^{-4}
Effective viscosity (kg/m-s)	0.05
Thermal diffusivity of solid (m ² /s)	3.3×10^{-5}
Thermal diffusivity of liquid (m ² /s)	7.5×10^{-5}
Specific heat of solid (J/kg-K)	710.6
Specific heat of liquid (J/kg-K)	836.0
Absorption coefficient	0.17
Temperature coefficient of surface tension (N/m-K)	-5.3×10^{-4}
Ratio of specific heats of vapor (γ_v)	1.667

Table 2— Enthalpies of Vaporization of the Alloying Elements^(a)

Element	Enthalpy (kJ/kg)
Iron	6087
Manganese	4005
Chromium	6577
Nickel	6388

(a) Ref. 27.

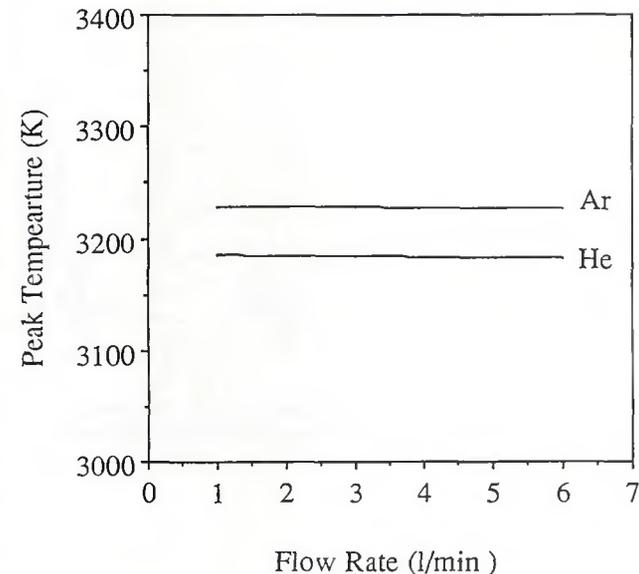


Fig. 9— Peak temperatures calculated as a function of gas flow rate and the type of the shielding gas used.

Table 3— Comparison of Predicted Values of Weld Pool Geometry and Peak Temperatures with Experimental Data for the Welding of AISI 202 Stainless Steel

Parameter	Experimental ^(a)	Model Prediction
Welding pool width (m)	8.2×10^{-4}	7.8×10^{-4}
Weld pool depth (m)	2.3×10^{-4}	2.0×10^{-4}
Peak temperatures (K)	3093 ± 44	3182

(a) Refs. 2, 15.

Table 4— Composition of the Alloying Elements in the AISI 202 Stainless Steel

Elements	Composition (wt-%)	Activity (mole fraction)
Manganese	6.58	0.066
Chromium	17.80	0.190
Nickel	4.77	0.045
Iron	70.14	0.698

steady state temperature and velocity fields, obtained from the solution of Navier-Stokes equations and the equations of conservation of mass and energy are shown in Fig. 3. The calculation takes into consideration the convective heat loss to the shielding gas and the evaporative heat loss at the pool surface in accordance with Equation 1. The data used for the calculations are presented in Tables 1 and 2. The details of the calculations of thermal diffusivity and viscosity of the shielding gas are presented in Appendix B. For low concentration of surface active elements, the temperature coefficient of surface tension is negative (Ref. 29). Therefore, the velocities at the weld pool surface, shown in Fig. 3, are radially outward re-

Table 5— Comparison of the Predicted Vapor Composition with the Experimentally Determined Values for the Welding of AISI 202 Stainless Steel

Composition Ratio (Moles of i/ Moles of j)	Experimental	Present Work
J_{Fe}/J_{Mn}	1.08 ± 0.07	1.00
J_{Cr}/J_{Mn}	0.56 ± 0.08	0.65
J_{Ni}/J_{Mn}	0.05 ± 0.01	0.05

sulting in a relatively shallow pool. The maximum radial velocity is of the order of 0.7 m/s, which is close to the value reported by Zacharia, et al. (Ref. 24). The computed strong temperature gradient on the surface of the pool is consistent with the absorption of a significant amount of energy in a small localized area near the laser beam axis. The theoretically predicted pool diameter and depth, presented in Table 3, were found to be in good agreement with the experimentally observed values (Refs. 2, 15). Furthermore, the theoretically predicted peak temperature indicated in Table 3 was found to be in good agreement with the temperature experimen-

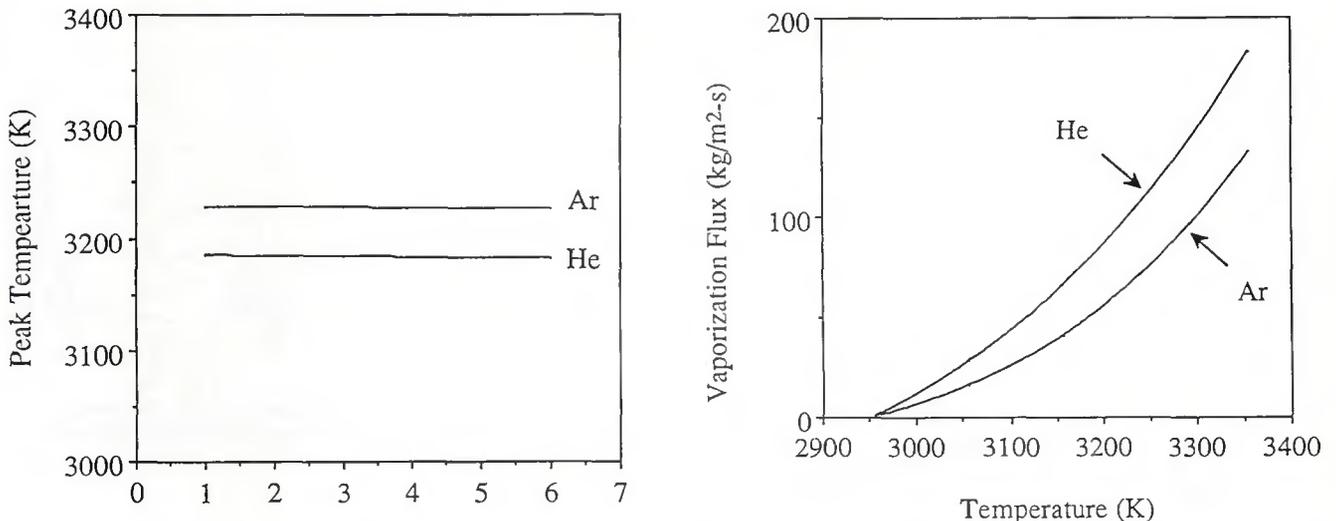


Fig. 10— Pressure gradient driven vaporization flux as function of temperature in helium and argon.

